

# Cubic Phase Light Emitters Hetero-integrated on Silicon

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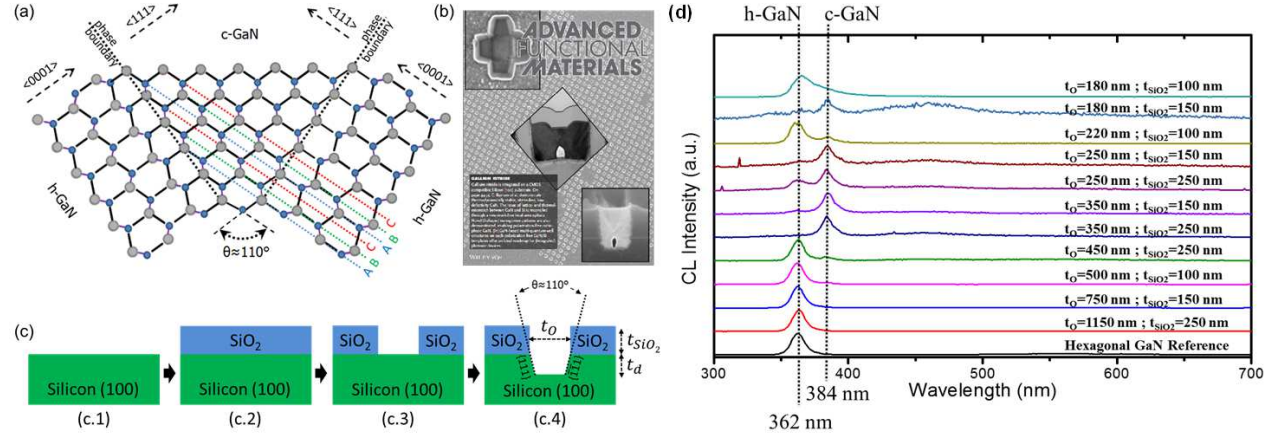
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**Abstract:** GaN emitters have historically been of hexagonal phase due to natural crystallization. Here we introduce a cubic phase GaN emitter technology that is polarization-free via co-integration on cheap and scalable CMOS-compatible Si(100) substrate.

**OCIS codes:** 230.0250; 230.3670; 310.3840; 250.5590; 160.6000

## 1. Introduction

Thanks to their direct bandgap across the entire visible spectrum and ultraviolet, Gallium Nitride (GaN) semiconductors and its compounds (AlGaInN) have transformed the visible light emitting diode industry and are now being explored for RF/power transistors. Almost without exception, GaN light emitting diodes (LEDs) (or any kind of GaN devices including RF/power transistors) are grown on three- or six-fold symmetry surfaces (e.g.  $\text{Al}_2\text{O}_3$ , SiC, Si(111) substrates) due to phase stability. The resulting GaN is therefore the six-fold symmetric hexagonal phase (wurtzite) GaN (h-GaN). The non-centrosymmetric nature (i.e. Ga and N atoms are not interchangeable in the lattice) of the hexagonal crystal arrangement leads to residual spontaneous and piezoelectric polarization fields. Both of these polarization fields are along the  $\langle 0001 \rangle$  growth direction, which is also the carrier injection direction in vertical transport devices, such as LEDs, lasers, and detectors, and thus are detrimental to recombination dynamics and device efficiency. On the other hand, cubic phase GaN (c-GaN) does not possess these polarization fields. Other advantages of c-GaN in photonic devices include cleavage planes and a higher optical gain. As such, there exists a need for a reliable approach for fabricating c-GaN for applications ranging from polarization-free photonics, normally-off transistors, room-temperature ferromagnetism, high-temperature spintronics, and single photon emitters. Yet, c-GaN is one of the least studied materials due to its phase instability and tendency to revert to the more stable h-GaN.



**Figure 1. A new method of cubic phase synthesis: Hexagonal-to-cubic transformation.** We report on the fundamental mechanisms in hexagonal-to-cubic phase transition in GaN hetero-integrated on a CMOS-compatible nano-patterned-Si (100) substrate. (a) We benefit from the crystallographic fact that hexagonal phase  $\langle 0001 \rangle$  direction is equivalent to the cubic phase  $\langle 111 \rangle$  direction. (b) Our recent cover article showing proof of concept feasibility in wurtzite-to-hexagonal transformation [1]. (c) Our process-flow (depicted as a cross-section) for U-shape grooved substrate preparation. (c.1) RCA cleaning, (c.2) Oxide ( $\text{SiO}_2$ ) growth, (c.3) Lithography and reactive ion etching of oxide ( $\text{SiO}_2$ ), (c.4) KOH dip (10%) to create the final groove structures of  $[\text{SiO}_2\text{-Si}\{111\}\text{-Si}\{100\}\text{-Si}\{111\}\text{-SiO}_2]$ . (d) Our recent works (under review) show distinct optical emission from h- and c- phase GaN at 362 nm (3.42 eV) and 384 nm (3.23 eV) at RT, respectively, showing the wurtzite-to-cubic phase transformation signature optically, for the very first time, by changing the nanopatterning parameters (i.e.  $t_0$  and  $t_{\text{SiO}_2}$ ) [2, 3].

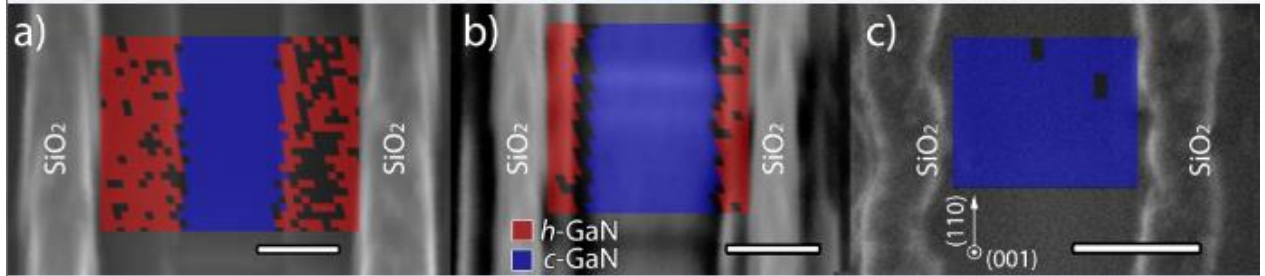
## 2. Approach

Conventional c-GaN is grown via planar epitaxy onto substrates such as GaAs, 3C-SiC, Si (100), and MgO, or via impurity incorporation. However, the c-GaN formed through these approaches suffers from high defectivity and phase mixing. Recently, c-GaN formation via phase transition on patterned substrates with V-shaped  $[\text{Si}\{111\}\text{-Si}\{111\}]$  or U-shaped  $[\text{Si}\{111\}\text{-Si}\{100\}\text{-Si}\{111\}]$  groove structures was introduced. Based on crystallographic geometry that h-crystal  $\langle 0001 \rangle$  direction and c-crystal  $\langle 111 \rangle$  direction are equivalent, it has been shown if two h-phase  $\langle 0001 \rangle$  growth fronts merge at an angle of  $\sim 109.5^\circ$  (i.e. the angle between the two Ga-N bonds in the

tetrahedral bonding), c-phase would form after the seam. Anisotropic nano-patterning of Si(100) substrates are typically used to create U-shaped (or V-shaped if etched all the way) grooves with a crystallographic angle of  $54.74^\circ$  between the (100) and (111)Si surfaces. Thus, GaN selective growth on Si(111) facets of a U-groove leads to two h-GaN growth fronts meeting at an angle of  $54.74^\circ \times 2 \approx 109.5^\circ$ , which is exactly the angle required to facilitate the transition of the h- GaN into c-GaN after coalescence.

### 3. Results and Discussion

Here we investigate the method of forming c-GaN in U-shaped grooves, propose a crystallographic model to describe the hexagonal-to-cubic phase transition in these grooves, and study the effects of nano-patterning parameters on c-GaN formation on CMOS-compatible Si(100). The most critical component of this approach is the substrate preparation with proper groove profile. We come up with a U-shaped, [SiO<sub>2</sub>-Si{111}-Si{100}-Si{111}-SiO<sub>2</sub>] groove structures for GaN-on-Si integration (see Figure 1c). The secret is the anisotropic etching of the Si (100) substrates which forms ideal angle of  $\sim 55^\circ$  on the (100)/(111) Si surfaces. Thus, when two wurtzite phase GaN growth fronts initiated from the Si {111} facets meet, the apex angle of  $\sim 110^\circ$  is achieved, transforming the wurtzite phase GaN into a cubic phase GaN after seam (as predicted by crystallographic theory in Fig. 1a). Extensive material characterizations including temperature-dependent cathodoluminescence, high resolution transmission electron microscopy, X-ray diffraction, selective area electron diffraction, electron backscattering, and photoluminescence have validated the experimental work [2, 3]. We recently demonstrated the optical quality of the layers via photoluminescence studies. Ultraviolet light emission from the cubic phase GaN on U-shaped grooved Si (100) substrate is achieved. Moreover, cubic phase InGaN/GaN multi-quantum-well active layers are grown on the cubic phase GaN/Si(100) and led to as-designed blue light emission.



**Figure 2. Top-view SEM images with EBSD overlay of polarization-free GaN emitters on a novel nano-grooved CMOS-compatible Si (100) substrate.** GaN on a U-grooves with (a) Partial (ff = 40%) c-GaN coverage, (b) Partial (ff = 65%) c-GaN coverage, and (c) Complete (ff  $\approx$  100%) c-GaN coverage. Each pixel has resolution of  $20 \times 20$  nm, and red, blue, grey colors correspond to h-GaN, c-GaN, and indistinguishable phases, respectively. The crystal orientation of c-GaN is identified and labelled in (c). The white scale bars in the bottom right of each figure correspond to 200 nm. [3]

### 4. Conclusion

Here we investigate the effects of nano-patterning parameters on cubic phase formation and demonstrate a method of forming pure cubic phase gallium nitride (GaN). First, U-shaped grooves with various patterning parameters are fabricated on CMOS-compatible Silicon (100) substrates. Next, metalorganic chemical vapor deposition is used to facilitate GaN growth in the grooves. Depending on the patterning parameters, a partial to complete hexagonal-to-cubic phase transition of GaN on the surface is reported. Finally, the resulting hexagonal and cubic phase materials are investigated via room (280 K) and low (5.7 K) temperature cathodoluminescence. A crystallographic model is proposed to explain the phase transition of GaN in such U-grooves. Experimental studies agree well with the crystallographic model, suggesting a relationship between GaN deposition thickness ( $h_c$ ), etch depth ( $t_d$ ), and opening width ( $p$ ) as  $h_c \approx 1.06p - 0.75t_d$  for complete cubic phase GaN surface coverage. Electron backscatter diffraction experiments validate single phase cubic GaN coverage that agrees well with the modelling. Moreover, we report on the additional benefits of this technology such as c-GaN on Si (100) has a natural cleavage plane – promising perfect mirror formation scheme for laser diode applications; is polarization-free so could be used as the gate for the design of normally-off GaN transistors, room-temperature ferromagnetism, high-temperature spintronics, single photon emitters; is CMOS compatible and scalable up-to 12 inch wafers.

### 5. References

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